Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 +)	-0.24	±0.09 (n=50)
logP (neutral XH)	2.63	±0.01 (n=50)
logP (X -)	0.46	
RMSD	0.266	

18C-09014 Points 2 to 24

M18_octanol concentration factor	0.988
Carbonate	0.1577 mM
Acidity error	-0.03698 mM

18C-09014 Points 25 to 48

M18_octanol concentration factor	0.944
Carbonate	0.1161 mM
Acidity error	-0.54687 mM

18C-09014 Points 49 to 73

M18_octanol concentration factor	0.993
Carbonate	0.1503 mM
Acidity error	-1.10219 mM

Warnings and errors

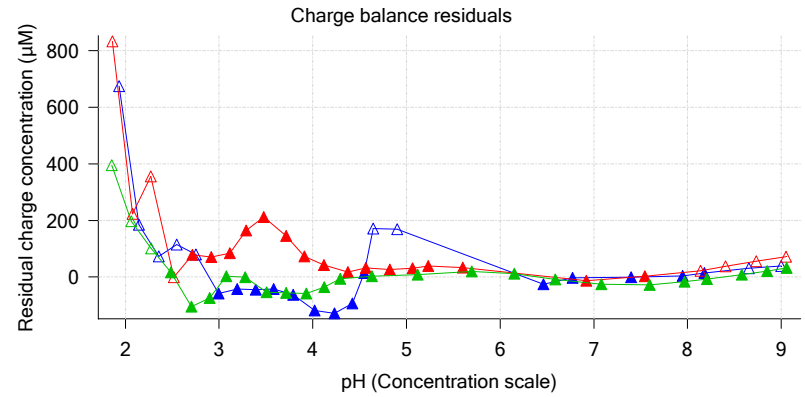
Errors	None
Warnings	None

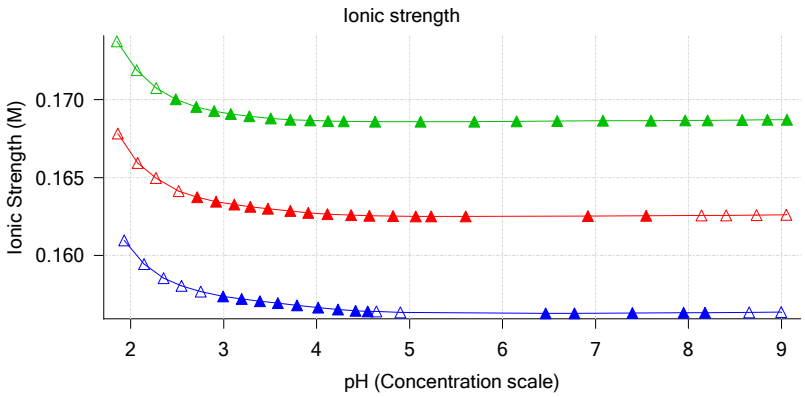
Sample logD and percent species

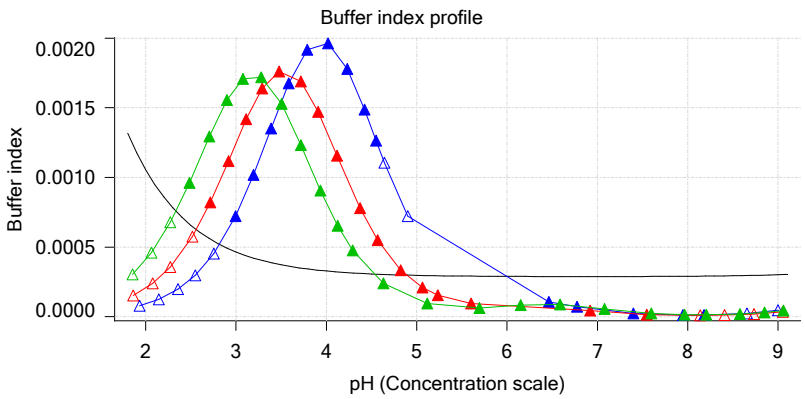
pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-0.23	63.00 %	0.00 %	0.00 %	35.85 %	1.14 %	0.00 %	
1.200	-0.22	62.58 %	0.00 %	0.00 %	35.61 %	1.80 %	0.00 %	Stomach pH
2.000	-0.12	57.11 %	0.02 %	0.00 %	32.50 %	10.37 %	0.00 %	
3.000	0.38	29.51 %	0.13 %	0.00 %	16.79 %	53.57 %	0.00 %	
4.000	1.25	5.06 %	0.22 %	0.00 %	2.88 %	91.85 %	0.00 %	
5.000	2.11	0.54 %	0.23 %	0.00 %	0.31 %	98.91 %	0.00 %	
6.000	2.54	0.05 %	0.23 %	0.00 %	0.03 %	99.68 %	0.00 %	
6.500	2.60	0.02 %	0.23 %	0.00 %	0.01 %	99.74 %	0.00 %	
7.000	2.62	0.01 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	
7.400	2.62	0.00 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	Blood pH
8.000	2.63	0.00 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	
9.000	2.62	0.00 %	0.23 %	0.01 %	0.00 %	99.75 %	0.02 %	
10.000	2.54	0.00 %	0.23 %	0.05 %	0.00 %	99.56 %	0.15 %	
11.000	2.13	0.00 %	0.23 %	0.51 %	0.00 %	97.77 %	1.48 %	
12.000	1.32	0.00 %	0.19 %	4.36 %	0.00 %	82.87 %	12.57 %	

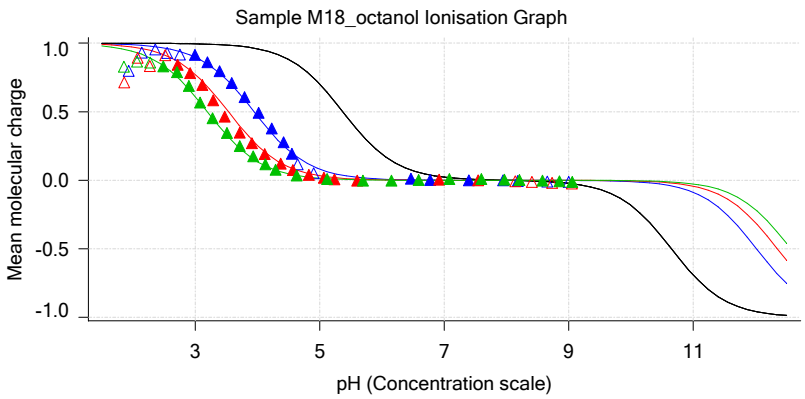
Sample name:	**M18_octanol**	Experiment start time:	**3/9/2018 8:37:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**		

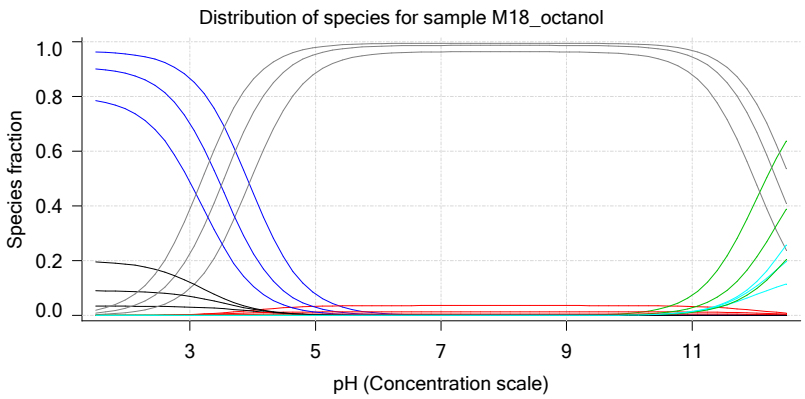
Graphs

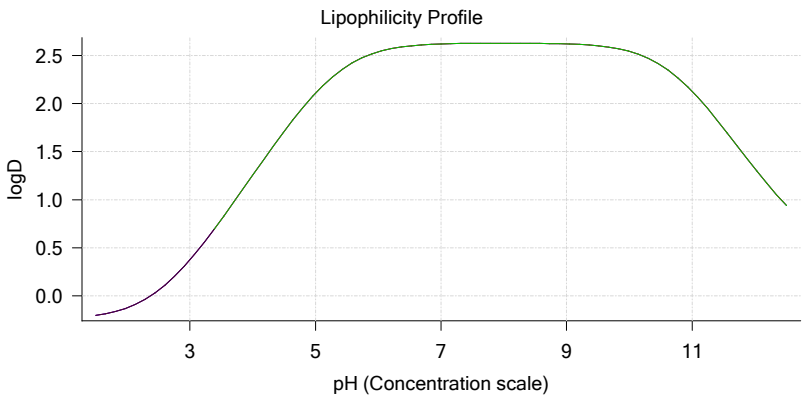


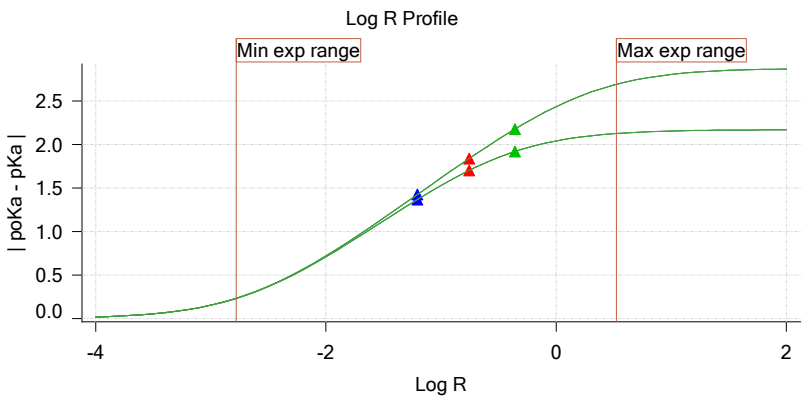


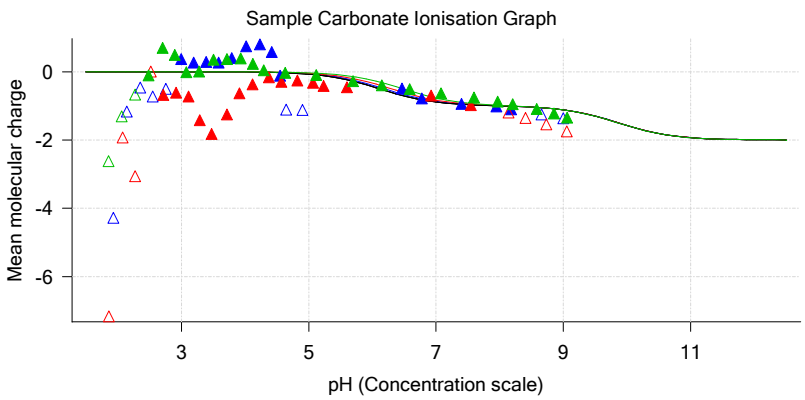








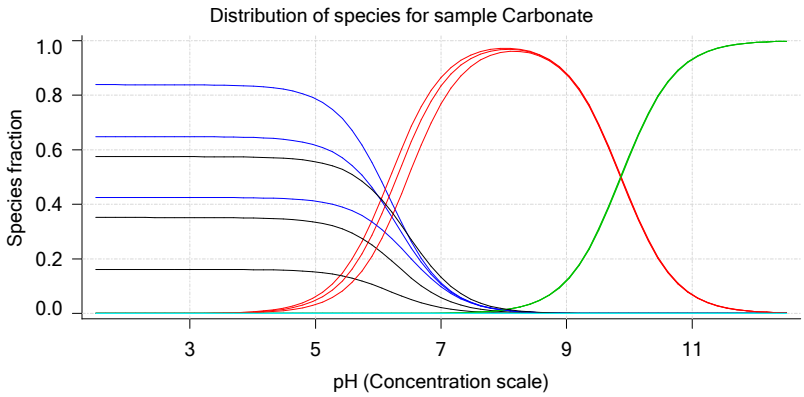




Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M18_octanol**	Experiment start time:	**3/9/2018 8:37:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-09014 Points 2 to 24

Overall results

RMSD	0.227
Average ionic strength	0.157 M
Average temperature	24.9°C
Partition ratio	0.0624 : 1
Analyte concentration range	3258.0 µM to 3348.4 µM
Total points considered	14 of 23

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.102	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r

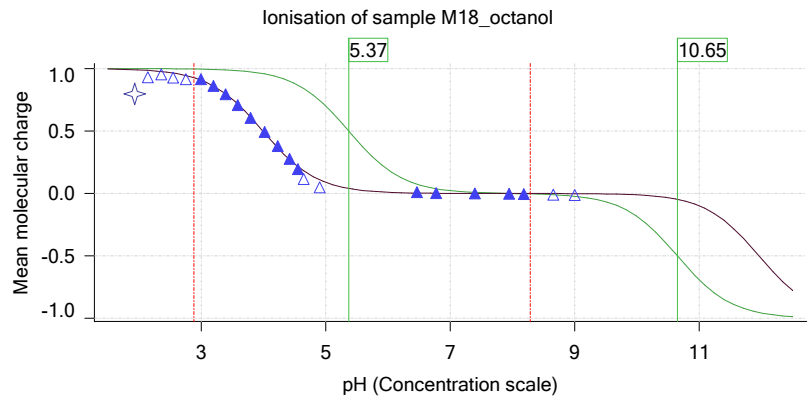
Titrants

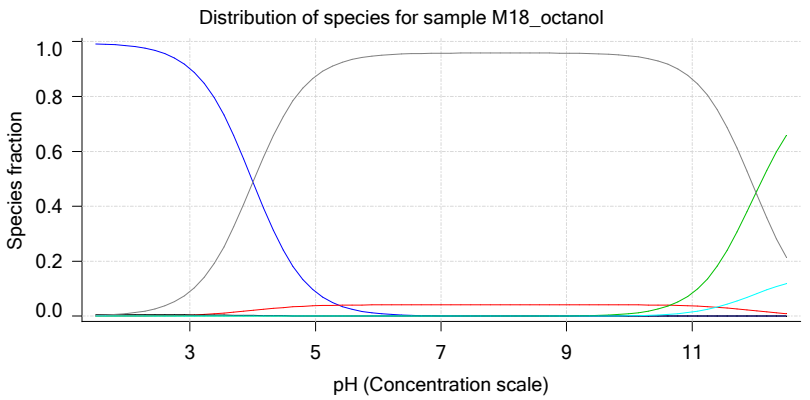
0.50 M HCl	0.999843	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 8:37:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor	0.988
Base pKa 1	5.37
Acid pKa 2	10.65
logP (XH2 +)	-1.08
logP (neutral XH)	2.57
logP (X -)	0.46

Sample graphs

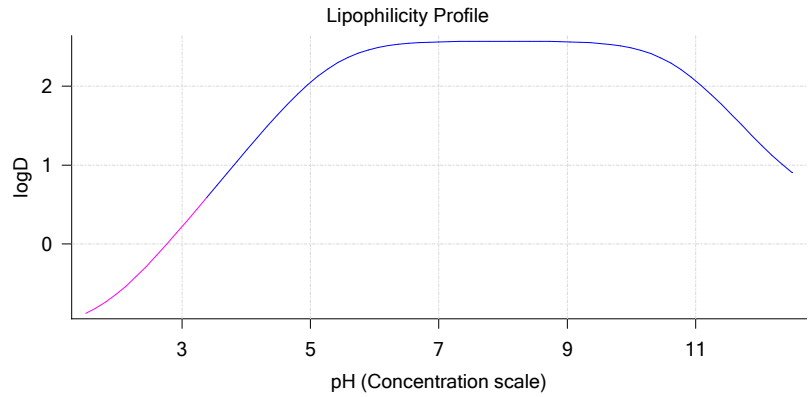




Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



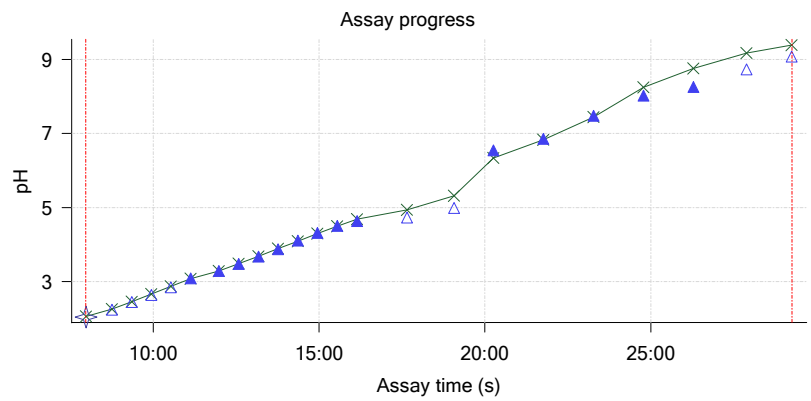
Sample logD and percent species

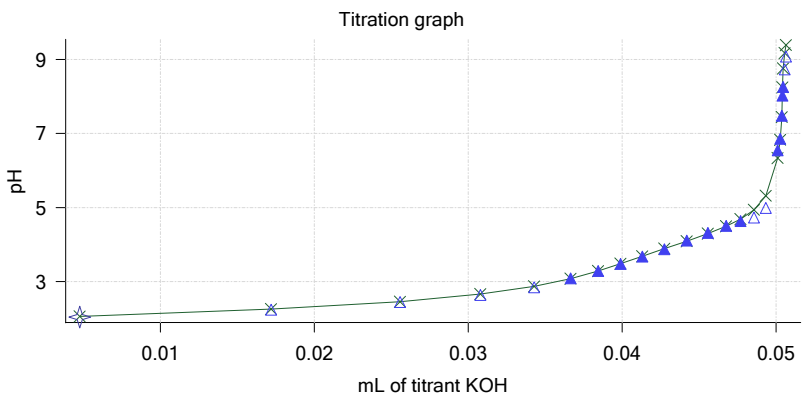
pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.01	99.39 %	0.00 %	0.00 %	0.51 %	0.10 %	0.00 %	
1.200	-0.97	99.33 %	0.01 %	0.00 %	0.51 %	0.16 %	0.00 %	Stomach pH
2.000	-0.62	98.48 %	0.04 %	0.00 %	0.51 %	0.97 %	0.00 %	
3.000	0.22	90.24 %	0.38 %	0.00 %	0.46 %	8.91 %	0.00 %	
4.000	1.18	49.14 %	2.10 %	0.00 %	0.25 %	48.51 %	0.00 %	
5.000	2.05	8.85 %	3.77 %	0.00 %	0.05 %	87.33 %	0.00 %	
6.000	2.48	0.96 %	4.10 %	0.00 %	0.00 %	94.93 %	0.00 %	
6.500	2.54	0.31 %	4.13 %	0.00 %	0.00 %	95.56 %	0.00 %	
7.000	2.56	0.10 %	4.14 %	0.00 %	0.00 %	95.76 %	0.00 %	
7.400	2.56	0.04 %	4.14 %	0.00 %	0.00 %	95.82 %	0.00 %	Blood pH
8.000	2.57	0.01 %	4.14 %	0.01 %	0.00 %	95.84 %	0.00 %	
9.000	2.56	0.00 %	4.14 %	0.09 %	0.00 %	95.75 %	0.02 %	
10.000	2.48	0.00 %	4.10 %	0.92 %	0.00 %	94.82 %	0.17 %	
11.000	2.07	0.00 %	3.73 %	8.36 %	0.00 %	86.40 %	1.50 %	
12.000	1.27	0.00 %	1.98 %	44.28 %	0.00 %	45.77 %	7.97 %	

Carbonate and acidity

Carbonate 0.158 mM
Acidity error -0.037 mM

Other graphs

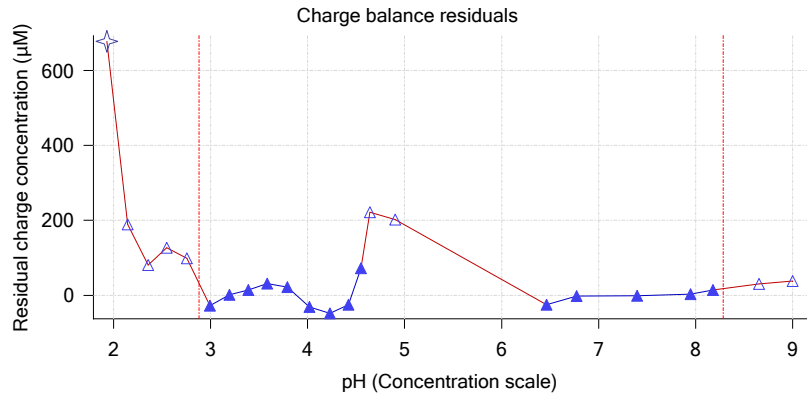


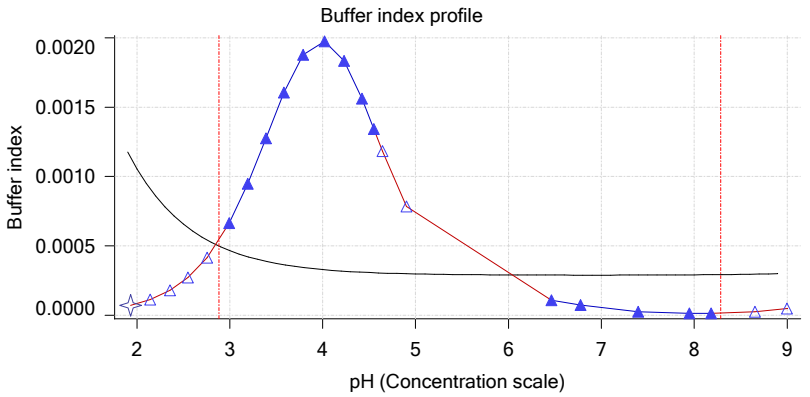


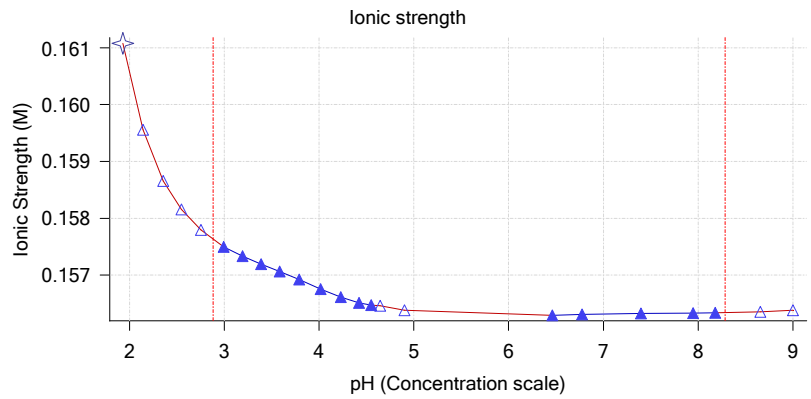
Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

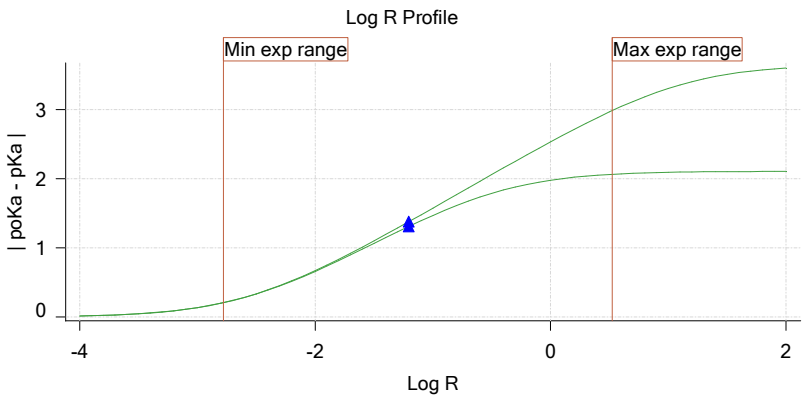
Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

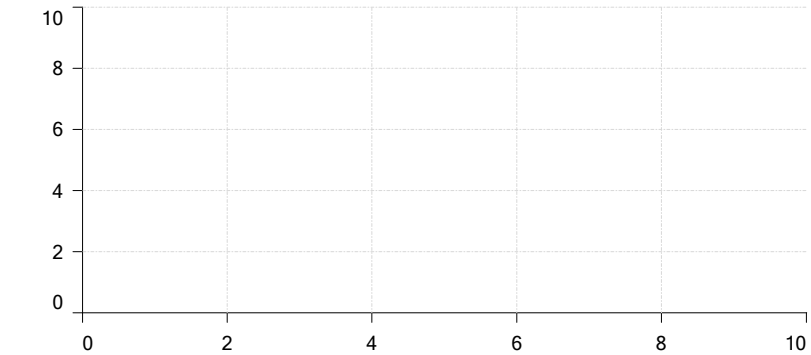
Other graphs (continued)

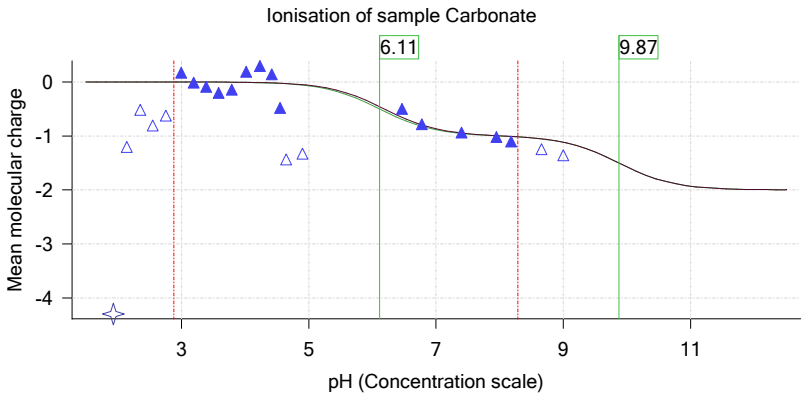












Sample name:	**M18_octanol**	Experiment start time:	**3/9/2018 8:37:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-09014 Points 25 to 48

Overall results

RMSD	0.131
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.1756 : 1
Analyte concentration range	2756.3 µM to 2832.3 µM
Total points considered	16 of 24

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.102	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r

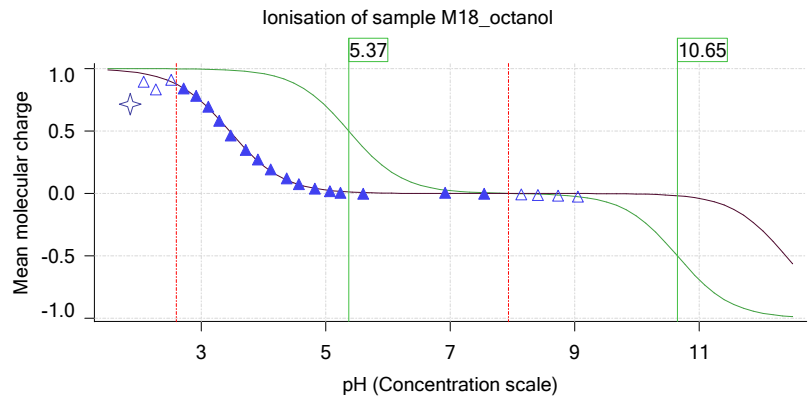
Titrants

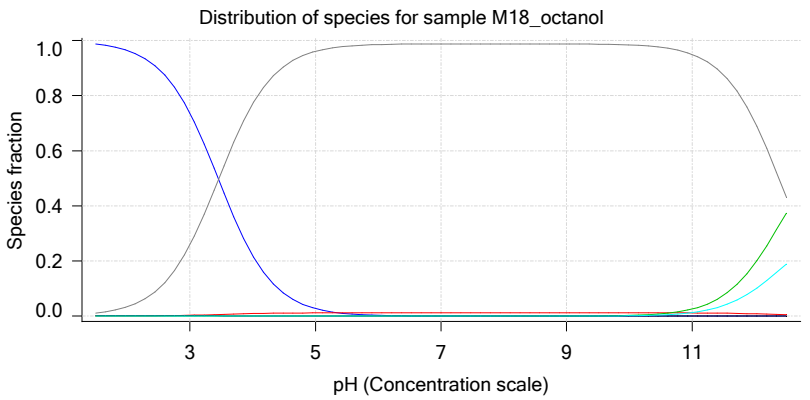
0.50 M HCl	0.999843	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 8:37:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor	0.944
Base pKa 1	5.37
Acid pKa 2	10.65
logP (XH2 +)	-1.92
logP (neutral XH)	2.67
logP (X -)	0.46

Sample graphs

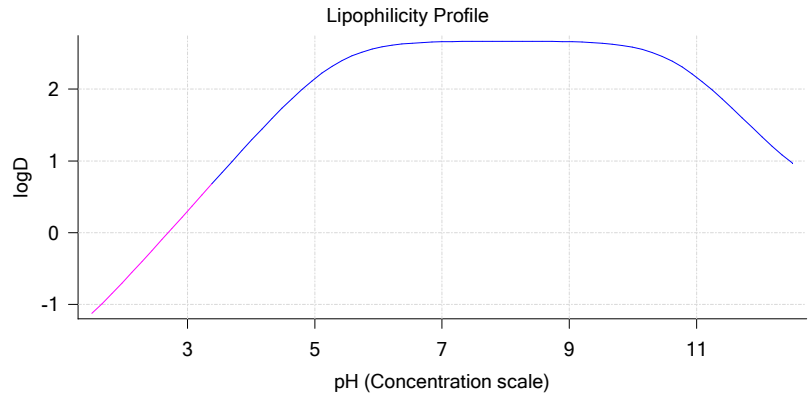




Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



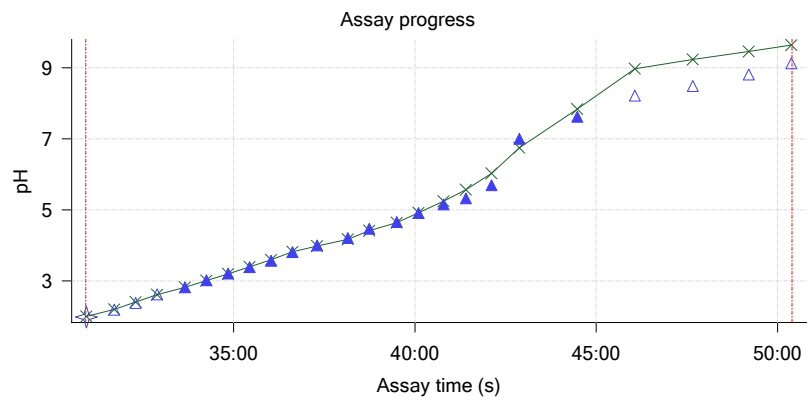
Sample logD and percent species

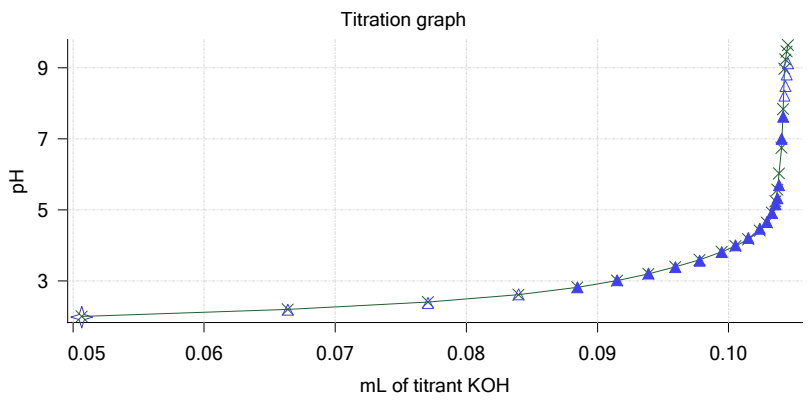
pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.50	99.44 %	0.00 %	0.00 %	0.21 %	0.35 %	0.00 %	
1.200	-1.36	99.23 %	0.01 %	0.00 %	0.21 %	0.55 %	0.00 %	Stomach pH
2.000	-0.68	96.38 %	0.04 %	0.00 %	0.20 %	3.37 %	0.00 %	
3.000	0.30	73.74 %	0.31 %	0.00 %	0.16 %	25.79 %	0.00 %	
4.000	1.28	22.02 %	0.94 %	0.00 %	0.05 %	76.99 %	0.00 %	
5.000	2.14	2.75 %	1.17 %	0.00 %	0.01 %	96.07 %	0.00 %	
6.000	2.58	0.28 %	1.20 %	0.00 %	0.00 %	98.52 %	0.00 %	
6.500	2.64	0.09 %	1.20 %	0.00 %	0.00 %	98.71 %	0.00 %	
7.000	2.66	0.03 %	1.20 %	0.00 %	0.00 %	98.77 %	0.00 %	
7.400	2.66	0.01 %	1.21 %	0.00 %	0.00 %	98.78 %	0.00 %	Blood pH
8.000	2.67	0.00 %	1.21 %	0.00 %	0.00 %	98.79 %	0.00 %	
9.000	2.66	0.00 %	1.20 %	0.03 %	0.00 %	98.75 %	0.01 %	
10.000	2.58	0.00 %	1.20 %	0.27 %	0.00 %	98.39 %	0.14 %	
11.000	2.16	0.00 %	1.16 %	2.59 %	0.00 %	94.94 %	1.31 %	
12.000	1.36	0.00 %	0.86 %	19.18 %	0.00 %	70.24 %	9.72 %	

Carbonate and acidity

Carbonate 0.116 mM
Acidity error -0.547 mM

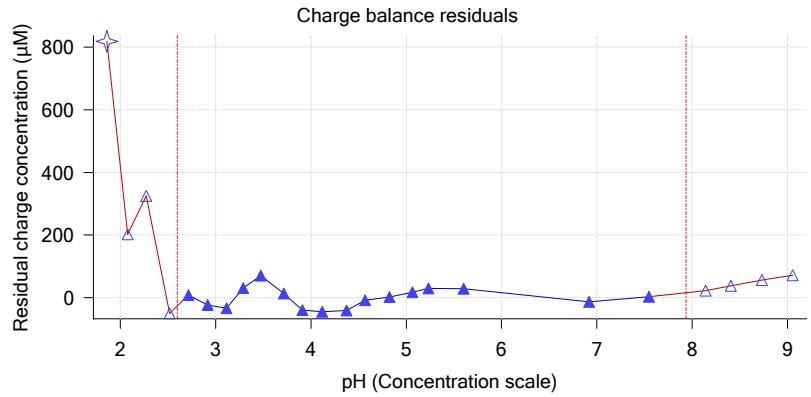
Other graphs

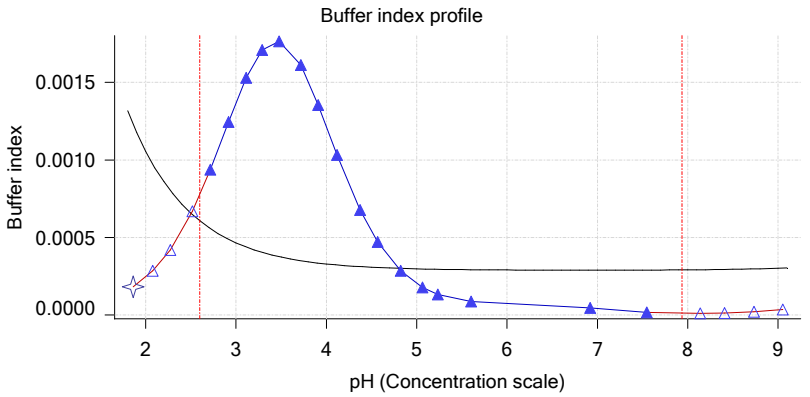


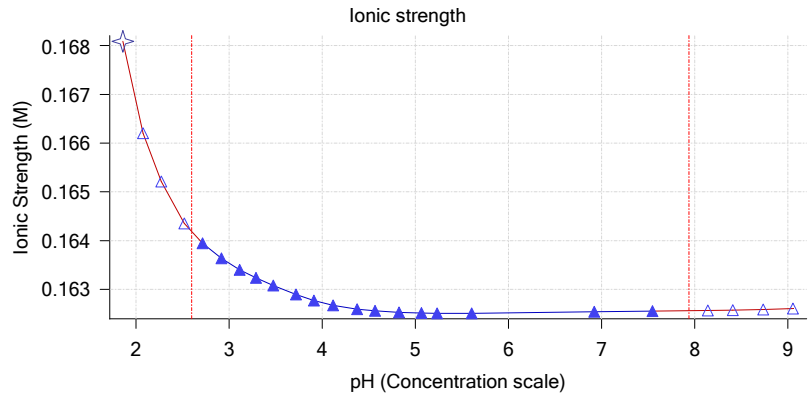


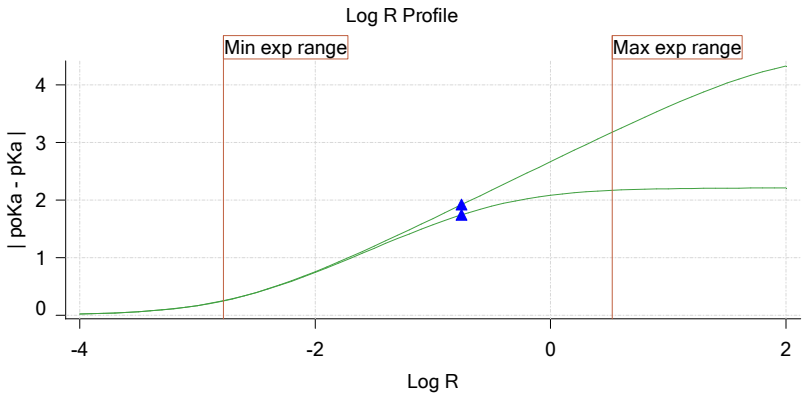
Sample name:	**M18_octanol**	Experiment start time:	**3/9/2018 8:37:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**		

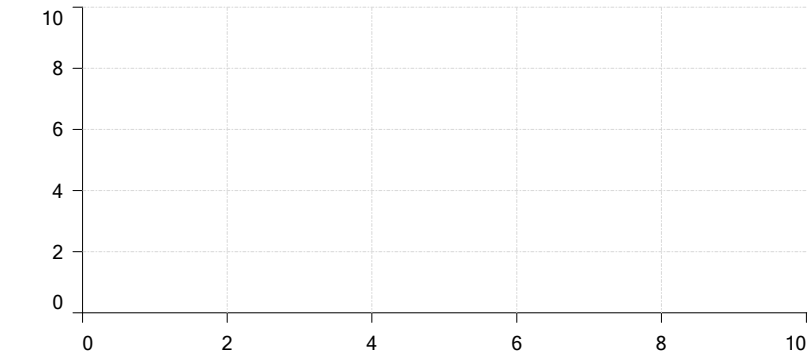
Other graphs (continued)

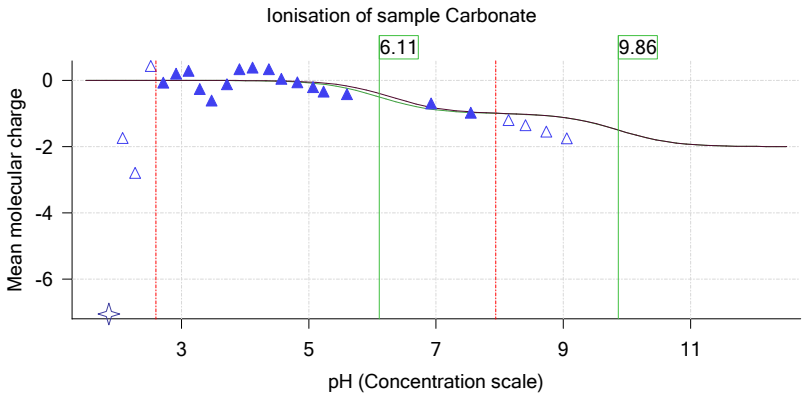












Sample name:	**M18_octanol**	Experiment start time:	**3/9/2018 8:37:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-09014 Points 49 to 73

Overall results

RMSD	0.342
Average ionic strength	0.169 M
Average temperature	25.0°C
Partition ratio	0.4375 : 1
Analyte concentration range	2105.7 µM to 2154.4 µM
Total points considered	22 of 25

Warnings and errors

Errors	None
Warnings	One or more logP values out of range
	Excessive acidity error present

Four-Plus parameters

Alpha	0.102	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r

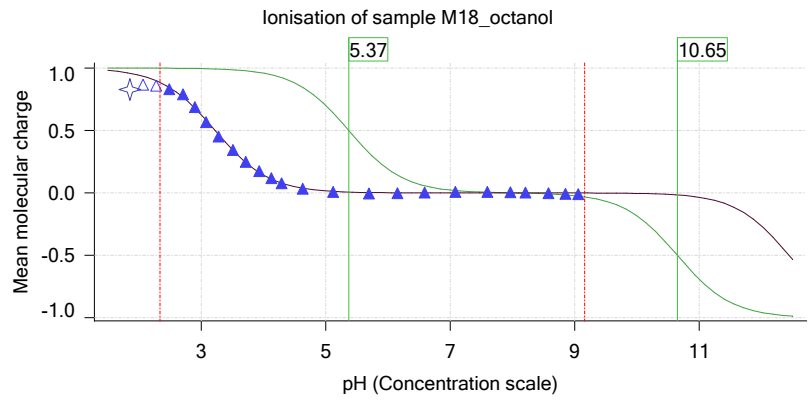
Titrants

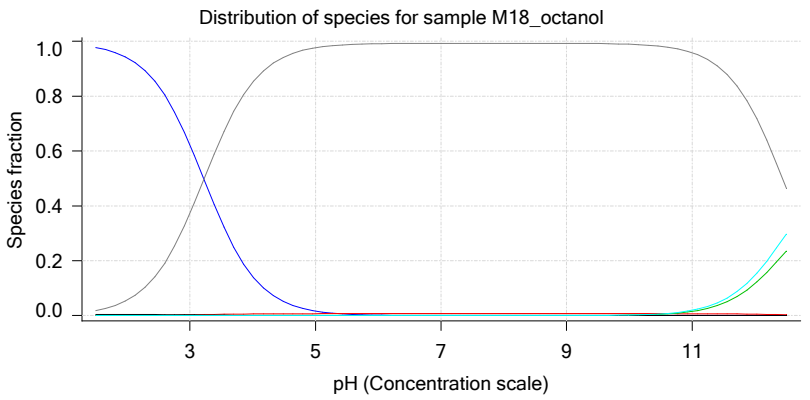
0.50 M HCl	0.999843	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 8:37:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor	0.993
Base pKa 1	5.37
Acid pKa 2	10.65
logP (XH2 +)	-2.03
logP (neutral XH)	2.50
logP (X -)	0.46

Sample graphs

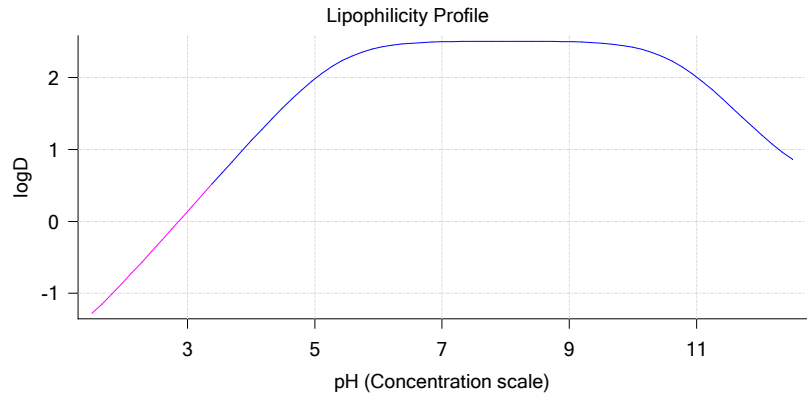




Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



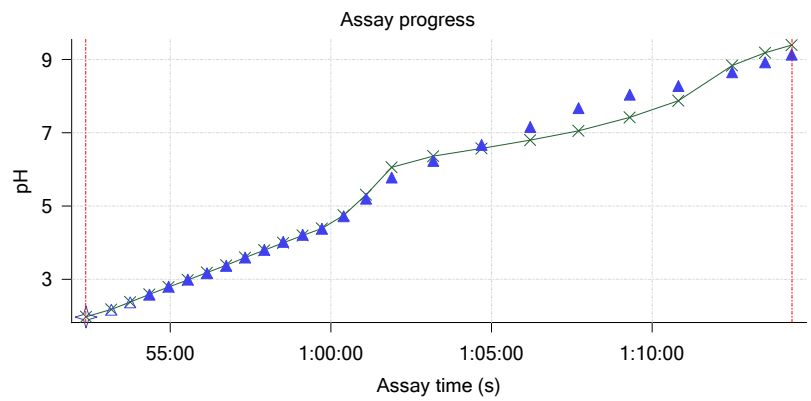
Sample logD and percent species

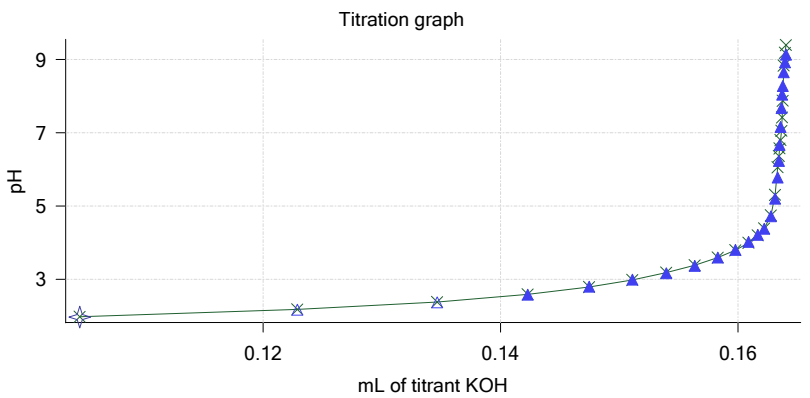
pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.64	99.00 %	0.00 %	0.00 %	0.40 %	0.59 %	0.00 %	
1.200	-1.51	98.66 %	0.01 %	0.00 %	0.40 %	0.93 %	0.00 %	Stomach pH
2.000	-0.84	93.97 %	0.04 %	0.00 %	0.38 %	5.61 %	0.00 %	
3.000	0.14	62.30 %	0.27 %	0.00 %	0.25 %	37.18 %	0.00 %	
4.000	1.12	14.25 %	0.61 %	0.00 %	0.06 %	85.08 %	0.00 %	
5.000	1.98	1.64 %	0.70 %	0.00 %	0.01 %	97.66 %	0.00 %	
6.000	2.41	0.17 %	0.71 %	0.00 %	0.00 %	99.12 %	0.00 %	
6.500	2.47	0.05 %	0.71 %	0.00 %	0.00 %	99.24 %	0.00 %	
7.000	2.49	0.02 %	0.71 %	0.00 %	0.00 %	99.27 %	0.00 %	
7.400	2.50	0.01 %	0.71 %	0.00 %	0.00 %	99.28 %	0.00 %	Blood pH
8.000	2.50	0.00 %	0.71 %	0.00 %	0.00 %	99.29 %	0.00 %	
9.000	2.50	0.00 %	0.71 %	0.02 %	0.00 %	99.25 %	0.02 %	
10.000	2.42	0.00 %	0.71 %	0.16 %	0.00 %	98.93 %	0.20 %	
11.000	2.00	0.00 %	0.69 %	1.53 %	0.00 %	95.85 %	1.93 %	
12.000	1.22	0.00 %	0.52 %	11.69 %	0.00 %	73.05 %	14.75 %	

Carbonate and acidity

Carbonate 0.150 mM
Acidity error -1.102 mM

Other graphs

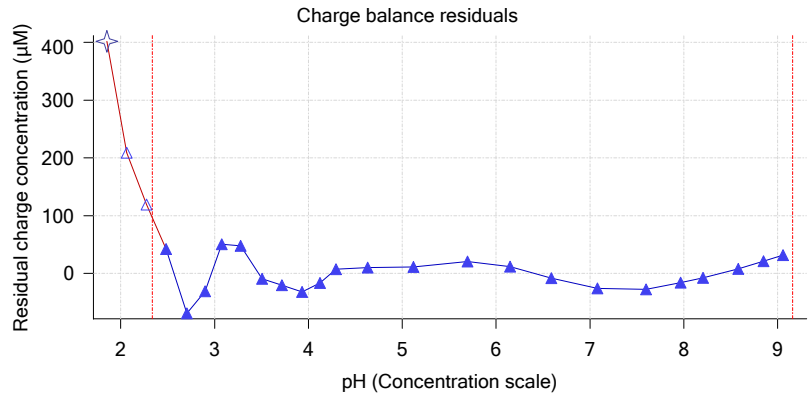


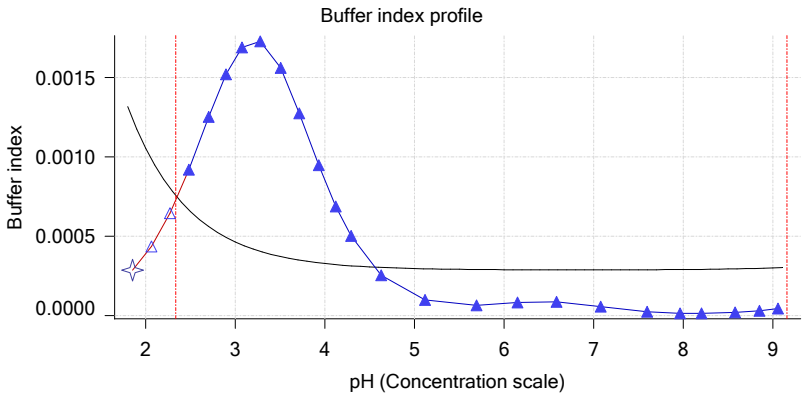


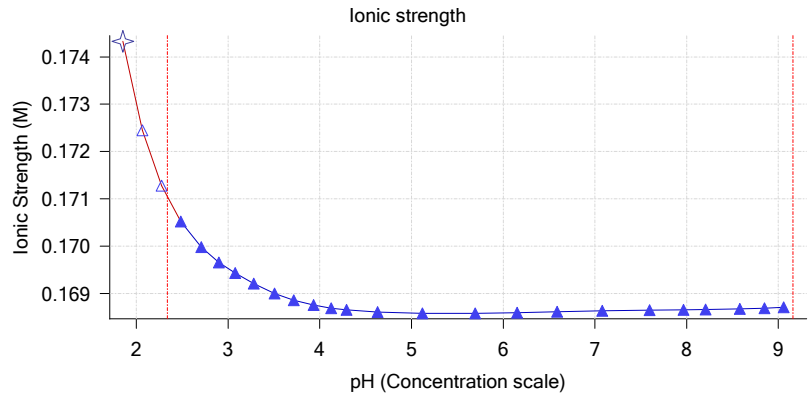
Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

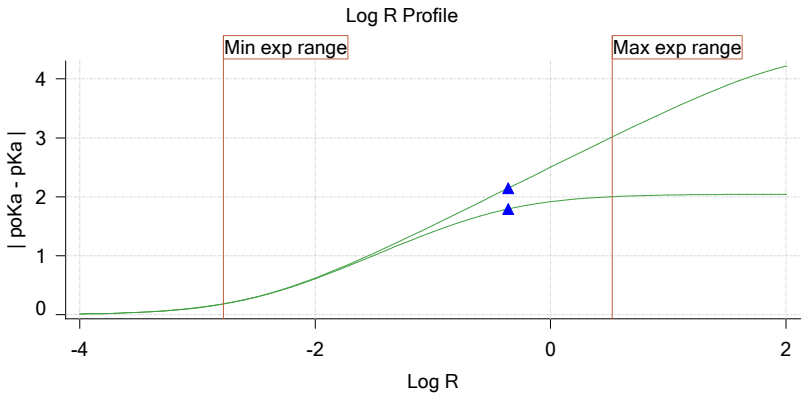
Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

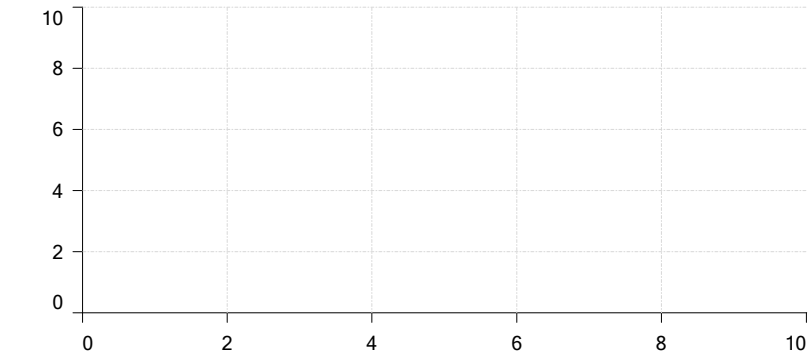
Other graphs (continued)

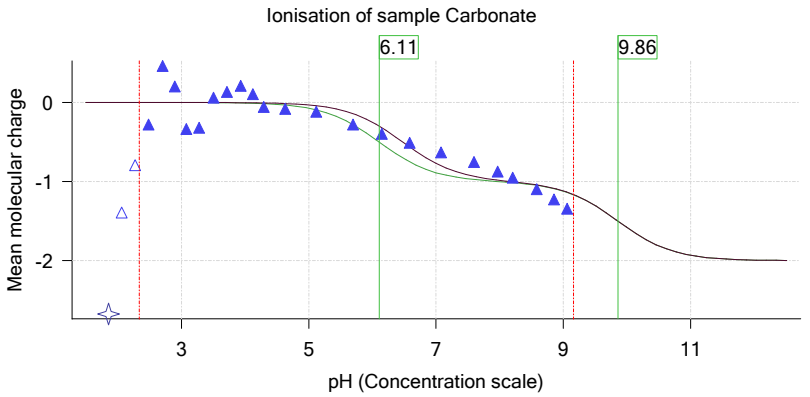












Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M18_octanol	2/27/2018 7:08:39 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001480 g	3/9/2018 2:22:36 PM	User entered value
Formula weight	267.11 g/mol	2/27/2018 7:08:39 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	267.11	2/27/2018 7:08:39 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 7:08:39 PM	User entered value
Sample is a	Ampholyte	2/27/2018 7:08:39 PM	User entered value
pKa 1	5.37	2/27/2018 7:08:39 PM	User entered value
Type	Base	2/27/2018 7:08:39 PM	User entered value
pKa 2	10.65	2/27/2018 7:08:39 PM	User entered value
Type	Acid	2/27/2018 7:08:39 PM	User entered value
logp (XH2 +)	-0.35	2/28/2018 3:20:28 PM	User entered value
logP (neutral XH)	2.57	3/2/2018 4:34:50 PM	User entered value
logP (X -)	0.46	2/27/2018 7:09:34 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dtime
4:57.9	Manual volume addition				0.10000 mL					
4:59.0	Initial pH = 7.17									
7:58.6	Data point 2	1.50000 mL	0.05002 mL	0.00475 mL	0.10000 mL	2.041	-0.00537	0.75188	0.00031	10.5 s
8:45.2	Data point 3	1.50000 mL	0.05002 mL	0.01719 mL	0.10000 mL	2.248	-0.00630	0.13591	0.00084	10.0 s
9:20.9	Data point 4	1.50000 mL	0.05002 mL	0.02556 mL	0.10000 mL	2.455	-0.00491	0.10647	0.00074	10.0 s
9:56.5	Data point 5	1.50000 mL	0.05002 mL	0.03079 mL	0.10000 mL	2.645	-0.00008	0.00076	0.00014	10.0 s
10:31.9	Data point 6	1.50000 mL	0.05002 mL	0.03429 mL	0.10000 mL	2.849	-0.00867	0.76331	0.00049	10.5 s
11:07.9	Data point 7	1.50000 mL	0.05002 mL	0.03667 mL	0.10000 mL	3.088	-0.00680	0.26943	0.00065	10.0 s
11:58.8	Data point 8	1.50000 mL	0.05002 mL	0.03845 mL	0.10000 mL	3.287	-0.00858	0.64011	0.00053	10.5 s
12:34.8	Data point 9	1.50000 mL	0.05002 mL	0.03991 mL	0.10000 mL	3.481	-0.00517	0.71303	0.00030	10.0 s
13:10.2	Data point 10	1.50000 mL	0.05002 mL	0.04132 mL	0.10000 mL	3.675	-0.01100	0.68415	0.00066	10.0 s
13:45.7	Data point 11	1.50000 mL	0.05002 mL	0.04276 mL	0.10000 mL	3.880	-0.01228	0.70505	0.00072	10.5 s
14:21.7	Data point 12	1.50000 mL	0.05002 mL	0.04421 mL	0.10000 mL	4.108	-0.01324	0.78765	0.00074	10.0 s
14:57.1	Data point 13	1.50000 mL	0.05002 mL	0.04558 mL	0.10000 mL	4.320	-0.00760	0.32722	0.00066	10.0 s
15:32.6	Data point 14	1.50000 mL	0.05002 mL	0.04675 mL	0.10000 mL	4.509	-0.01875	0.88887	0.00098	10.5 s
16:08.5	Data point 15	1.50000 mL	0.05002 mL	0.04770 mL	0.10000 mL	4.638	-0.09531	0.99824	0.00471	Timed out at
17:39.0	Data point 16	1.50000 mL	0.05002 mL	0.04857 mL	0.10000 mL	4.731	-0.03485	0.99545	0.00173	Timed out at
19:04.3	Data point 17	1.50000 mL	0.05002 mL	0.04934 mL	0.10000 mL	4.989	-0.01963	0.98594	0.00098	40.5 s

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
20:15.5	Data point 18	1.50000 mL	0.05002 mL	0.05012 mL	0.10000 mL	6.544	-0.03976	0.99389	0.00197	Timed out at 59.5 s
21:46.0	Data point 19	1.50000 mL	0.05002 mL	0.05028 mL	0.10000 mL	6.855	-0.03344	0.99646	0.00165	Timed out at 59.5 s
23:16.5	Data point 20	1.50000 mL	0.05002 mL	0.05038 mL	0.10000 mL	7.476	-0.05450	0.99713	0.00270	Timed out at 59.5 s
24:47.0	Data point 21	1.50000 mL	0.05002 mL	0.05042 mL	0.10000 mL	8.023	-0.06285	0.99743	0.00311	Timed out at 59.5 s
26:17.5	Data point 22	1.50000 mL	0.05002 mL	0.05047 mL	0.10000 mL	8.256	-0.04162	0.99520	0.00206	Timed out at 59.5 s
27:53.2	Data point 23	1.50000 mL	0.05002 mL	0.05056 mL	0.10000 mL	8.730	-0.01987	0.99215	0.00099	51.0 s
29:14.8	Data point 24	1.50000 mL	0.05002 mL	0.05066 mL	0.10000 mL	9.072	-0.01966	0.96316	0.00099	38.5 s
30:56.2	Data point 25	1.50000 mL	0.10564 mL	0.05066 mL	0.30000 mL	1.973	-0.00826	0.81865	0.00045	10.0 s
31:42.4	Data point 26	1.50000 mL	0.10564 mL	0.06639 mL	0.30000 mL	2.182	-0.00740	0.49850	0.00052	10.0 s
32:18.0	Data point 27	1.50000 mL	0.10564 mL	0.07707 mL	0.30000 mL	2.373	-0.00564	0.17659	0.00066	10.0 s
32:53.6	Data point 28	1.50000 mL	0.10564 mL	0.08398 mL	0.30000 mL	2.615	0.00002	0.00001	0.00050	10.0 s
33:39.6	Data point 29	1.50000 mL	0.10564 mL	0.08848 mL	0.30000 mL	2.812	-0.00441	0.74067	0.00025	10.0 s
34:15.1	Data point 30	1.50000 mL	0.10564 mL	0.09151 mL	0.30000 mL	3.012	-0.01157	0.77811	0.00065	10.5 s
34:51.1	Data point 31	1.50000 mL	0.10564 mL	0.09389 mL	0.30000 mL	3.207	-0.00365	0.80988	0.00020	10.0 s
35:26.5	Data point 32	1.50000 mL	0.10564 mL	0.09593 mL	0.30000 mL	3.381	-0.00664	0.44901	0.00049	10.0 s
36:01.9	Data point 33	1.50000 mL	0.10564 mL	0.09779 mL	0.30000 mL	3.567	-0.01484	0.65999	0.00090	10.0 s
36:37.4	Data point 34	1.50000 mL	0.10564 mL	0.09948 mL	0.30000 mL	3.807	-0.00593	0.14880	0.00076	10.0 s
37:18.0	Data point 35	1.50000 mL	0.10564 mL	0.10052 mL	0.30000 mL	3.999	-0.00035	0.00113	0.00051	10.0 s
38:08.9	Data point 36	1.50000 mL	0.10564 mL	0.10151 mL	0.30000 mL	4.207	-0.00527	0.79747	0.00029	10.0 s
38:44.4	Data point 37	1.50000 mL	0.10564 mL	0.10237 mL	0.30000 mL	4.462	-0.00775	0.68238	0.00046	10.0 s
39:30.1	Data point 38	1.50000 mL	0.10564 mL	0.10292 mL	0.30000 mL	4.655	-0.00577	0.49479	0.00040	10.5 s
40:06.0	Data point 39	1.50000 mL	0.10564 mL	0.10332 mL	0.30000 mL	4.910	-0.01228	0.58176	0.00079	10.5 s
40:47.1	Data point 40	1.50000 mL	0.10564 mL	0.10358 mL	0.30000 mL	5.151	-0.01553	0.76936	0.00087	12.0 s
41:24.5	Data point 41	1.50000 mL	0.10564 mL	0.10372 mL	0.30000 mL	5.319	-0.01184	0.46775	0.00086	11.5 s
42:06.6	Data point 42	1.50000 mL	0.10564 mL	0.10386 mL	0.30000 mL	5.687	-0.01865	0.92517	0.00096	15.5 s
42:52.8	Data point 43	1.50000 mL	0.10564 mL	0.10405 mL	0.30000 mL	7.000	-0.08496	0.99448	0.00421	Timed out at 59.5 s
44:28.4	Data point 44	1.50000 mL	0.10564 mL	0.10416 mL	0.30000 mL	7.624	-0.06603	0.99772	0.00326	Timed out at 59.5 s
46:04.1	Data point 45	1.50000 mL	0.10564 mL	0.10426 mL	0.30000 mL	8.216	-0.04320	0.99574	0.00214	Timed out at 59.5 s
47:39.9	Data point 46	1.50000 mL	0.10564 mL	0.10433 mL	0.30000 mL	8.482	-0.01966	0.98330	0.00098	57.0 s
49:12.6	Data point 47	1.50000 mL	0.10564 mL	0.10442 mL	0.30000 mL	8.807	-0.02001	0.98580	0.00100	40.0 s
50:23.1	Data point 48	1.50000 mL	0.10564 mL	0.10454 mL	0.30000 mL	9.125	-0.01779	0.90618	0.00092	34.5 s
52:23.2	Data point 49	1.50000 mL	0.16729 mL	0.10454 mL	0.80000 mL	1.966	-0.01371	0.95560	0.00069	10.5 s
53:10.0	Data point 50	1.50000 mL	0.16729 mL	0.12288 mL	0.80000 mL	2.170	0.00380	0.50246	0.00026	10.0 s
53:45.8	Data point 51	1.50000 mL	0.16729 mL	0.13467 mL	0.80000 mL	2.375	0.01474	0.76262	0.00083	10.0 s
54:21.4	Data point 52	1.50000 mL	0.16729 mL	0.14229 mL	0.80000 mL	2.582	-0.00433	0.22604	0.00045	10.0 s
54:56.9	Data point 53	1.50000 mL	0.16729 mL	0.14746 mL	0.80000 mL	2.802	-0.01110	0.57112	0.00072	10.5 s
55:32.9	Data point 54	1.50000 mL	0.16729 mL	0.15110 mL	0.80000 mL	2.992	-0.00395	0.04126	0.00096	10.5 s
56:09.0	Data point 55	1.50000 mL	0.16729 mL	0.15398 mL	0.80000 mL	3.169	0.00169	0.00837	0.00091	10.0 s
56:44.4	Data point 56	1.50000 mL	0.16729 mL	0.15637 mL	0.80000 mL	3.371	-0.00442	0.51991	0.00030	10.0 s
57:20.0	Data point 57	1.50000 mL	0.16729 mL	0.15832 mL	0.80000 mL	3.598	-0.00476	0.13870	0.00063	10.5 s
57:55.8	Data point 58	1.50000 mL	0.16729 mL	0.15981 mL	0.80000 mL	3.807	-0.00790	0.80262	0.00044	10.0 s
58:31.3	Data point 59	1.50000 mL	0.16729 mL	0.16091 mL	0.80000 mL	4.022	0.00289	0.02519	0.00090	10.5 s
59:07.2	Data point 60	1.50000 mL	0.16729 mL	0.16169 mL	0.80000 mL	4.213	0.00323	0.17283	0.00038	10.5 s
59:43.0	Data point 61	1.50000 mL	0.16729 mL	0.16223 mL	0.80000 mL	4.381	-0.00427	0.08186	0.00074	10.5 s
1:00:24.2	Data point 62	1.50000 mL	0.16729 mL	0.16279 mL	0.80000 mL	4.718	-0.01425	0.87866	0.00075	11.0 s
1:01:05.7	Data point 63	1.50000 mL	0.16729 mL	0.16315 mL	0.80000 mL	5.204	-0.00635	0.10706	0.00096	12.0 s
1:01:53.3	Data point 64	1.50000 mL	0.16729 mL	0.16336 mL	0.80000 mL	5.779	-0.01830	0.86406	0.00097	47.0 s
1:03:10.9	Data point 65	1.50000 mL	0.16729 mL	0.16345 mL	0.80000 mL	6.233	-0.02014	0.98026	0.00100	Timed out at 59.5 s

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09014**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09014_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:04:41.4	Data point 66	1.50000 mL	0.16729 mL	0.16352 mL	0.80000 mL	6.668	-0.04896	0.99508	0.00242	Timed out at 59.5 s
1:06:12.0	Data point 67	1.50000 mL	0.16729 mL	0.16359 mL	0.80000 mL	7.159	-0.06899	0.99765	0.00341	Timed out at 59.5 s
1:07:42.4	Data point 68	1.50000 mL	0.16729 mL	0.16366 mL	0.80000 mL	7.675	-0.06553	0.99682	0.00324	Timed out at 59.5 s
1:09:18.0	Data point 69	1.50000 mL	0.16729 mL	0.16373 mL	0.80000 mL	8.043	-0.04078	0.98943	0.00202	Timed out at 59.5 s
1:10:48.5	Data point 70	1.50000 mL	0.16729 mL	0.16378 mL	0.80000 mL	8.282	-0.02444	0.97943	0.00122	Timed out at 59.5 s
1:12:29.2	Data point 71	1.50000 mL	0.16729 mL	0.16388 mL	0.80000 mL	8.654	-0.01571	0.67890	0.00094	25.5 s
1:13:30.4	Data point 72	1.50000 mL	0.16729 mL	0.16397 mL	0.80000 mL	8.923	-0.00987	0.25217	0.00097	14.0 s
1:14:20.0	Data point 73	1.50000 mL	0.16729 mL	0.16406 mL	0.80000 mL	9.132	-0.01934	0.95656	0.00098	25.0 s
1:14:54.1	Assay volumes	1.50000 mL	0.16729 mL	0.16406 mL	0.80000 mL					

Sample name: **M18_octanol**
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Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.100 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M18_octanol**
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Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.500 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.102	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus S	0.9967	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jH	1.2	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jOH	0.0	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r
Base concentration factor	1.000	3/9/2018 8:37:21 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	1.000	3/9/2018 8:37:21 PM	C:\Sirius_T3\HCl18C09.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 11:05:59 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 11:27:22 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 11:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M18_octanol**
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Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titrator		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+5.00 mV		3/9/2018 8:37:49 PM
Filling solution	3M KCl	KCL097	3/9/2018 11:05:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/9/2018 11:04:22 AM
Wash 2	0.5% Trition X-100 in H20		3/9/2018 11:04:25 AM
Buffer position 1	pH7 Wash		3/9/2018 11:04:27 AM
Buffer position 2	pH 7		3/9/2018 11:04:30 AM
Storage position			3/9/2018 11:05:04 AM
Wash water	5.1e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	1e+004 mL		11/28/2017 11:36:29 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	123:16:41		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

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Experiment start time: **3/9/2018 8:37:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00